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Lattice Chiral Symmetry, Topology, Flux Tubes, Algorithms and Machines: The NIC Research Group Elementary Particle Physics

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We discuss the activities of the NIC research group elementary particle physics. Topics are chiral invariant formulations of lattice fermions, flux tube models, results relevant for phenomenology and the interpretation of experimental data, and algorithms and machines.

1 Introduction

No doubt, the existing models of the fundamental forces between elementary particles are very successful. The predictions of the electroweak Standard model were tested with striking success at accelerators worldwide. Quantum Chromo Dynamics (QCD) as our theory of the strong interactions is also well tested to a high precision for processes with a large momentum transfer. The only exception, where we do not have a satisfactory framework for a quantum theory is the gravitational force which remains a major challenge for elementary particle theory. The theoretical tool to describe elementary particle interactions are quantum field theories with the construction principle of local gauge invariance.

The main method to analyze these models is perturbation theory which performs an expansion in the coupling of the theory, assuming its value to be sufficiently small. While the calculations within perturbation theory have entered a level where very precise multi-loop orders are reached, there are phenomena that can not be addressed by perturbation theory, leaving many open questions such as: Why are quarks confined? Why is the binding energy of hadrons so enormously large? [a] What is the mechanism of breaking the fundamental chiral symmetry of QCD that leads to the light meson spectrum observed? What is the nature of the finite temperature QCD phase transition and what are the properties of the quark gluon plasma that existed shortly after the big bang? What is the nature of CP-violation? This list of questions is by far not exhausting and could be extended easily.

The problem is that the above questions are of inherent non-perturbative nature and answers can only be found by employing methods that extend well beyond perturbation theory. Such a method –which is the only one we know of today– is lattice field theory[1]. In the lattice approach our usual space-time is made discrete and a non-vanishing value of a lattice spacing a is introduced. Working with finite physical volumes, the continuum space-time on which the quantum field theories are defined, can be transformed into a discrete set of lattice points and the problem can be mapped to a computer code.

[a] The mass of the constituent quarks of a proton is a few MeV while the proton's mass is about a factor of 100 larger!

This allows then for first principle calculations of physical observables having as only input a given theoretical model. Of course, the discreteness of the space-time structure is only an approximation to the real world and eventually this systematic error has to be removed through a well-controlled continuum limit where the lattice spacing a is sent to zero. The computer evaluation of the models of elementary particle physics are performed with the help of Monte Carlo methods, computing by importance sampling the underlying Boltzmann distribution of the model of interest. Typical such simulation methods are the Metropolis, heat bath, cluster and molecular dynamics algorithms (see the books[2–5] for general introductions to lattice gauge theory).

In present lattice simulations we make use of a number of theoretical developments that helped us to understand how to control systematic errors such as discretization effects, non-perturbative renormalization, finite size effects and chiral symmetry violations. Unfortunately, such simulations demand enormous computer power and state of the art, high-end supercomputers have to be employed to solve the highly non-linear equations that appear in the physics problems (see the annual international lattice symposia[6]).

In the following we give a few examples of problems that are addressed in the NIC research group elementary particle physics.

2 Chiral Invariant Formulation of QCD

Chiral symmetry, the interchange of left and right-handed massless particles, is an important concept in continuum QCD where, through spontaneous symmetry breaking, it leads to the observed spectrum of the light mesons. One way to express chiral symmetry is that the Dirac operator $D_{\rm cont}$ anti-commutes with $\gamma_5 = \mathrm{diag}(1, 1, -1, -1)$, i.e. $\gamma_5 D_{\rm cont} + D_{\rm cont}\gamma_5 = 0$. Chiral eigenstates are then eigenstates of γ_5 with either positive chirality (right-handed particles) or negative chirality (left-handed particles). On the lattice, the concept of chiral symmetry appears to be be difficult to realize and since the invention of lattice field theory in 1974[1], no satisfactory solution could be found (see, e.g. Ref. 7 for a discussion of this topic).

A change of this situation occurred with the rediscovery[8] of the Ginsparg-Wilson[9] relation which reads for some lattice Dirac operator D,

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D \; . \tag{1}$$

Clearly, in the limit that the lattice spacing a vanishes the usual anti-commutation relation of the continuum Dirac operator is recovered. The Ginsparg-Wilson relation implies an exact lattice chiral symmetry[10] if the action used is constructed with a lattice Dirac operator that solves the Ginsparg-Wilson relation. The modification compared to the continuum is that γ_5 is replaced by $\gamma_5 \cdot (1 - a/2D)$. In general, an operator that satisfies the Ginsparg-Wilson relation on the lattice leads to properties of the corresponding lattice theory that are very similar to the continuum target theory. Thus, "Ginsparg-Wilson fermions" are an important conceptual tool for investigating non-perturbative aspects of physics. At present, also a number of lattice simulations have been performed with chiral invariant formulations of lattice QCD and questions of QCD are addressed that could not be explored before (see the reviews 11–13). Examples are the ϵ-regime of chiral perturbation theory and random matrix theory, see also Ref. 14 and the contribution to this proceedings[15] and references therein.

Another important aspect where Ginsparg-Wilson fermions become especially important is the role of topology. The mediators of the forces between the quarks are the gluons, which are represented as gauge fields in QCD. These gauge fields can be classified to belong to different topological sectors, having different topological charge ("winding numbers"). The topology of the gauge fields can be connected to semi-classical objects such as instantons[16], lumps[17] or so-called Kraan-van Baal[18] solutions. Such objects can be interpreted to play an important role, or are even responsible, for the confinement mechanism or chiral symmetry breaking.

On the lattice, it has been notoriously difficult to determine the topology of a lattice gauge field. Different methods lead to different results, rendering an investigation of the importance and the role of topology and semi-classical objects to be very cumbersome. Conceptually, the Atiyah-Singer index theorem[19] allows for a sound definition of the topological charge from the difference of the zero modes with positive and negative chirality.

Such a definition requires, however, obviously a notion of chirality on the lattice, a concept that only became possible with Ginsparg-Wilson fermions. Indeed, in practical simulations, chiral zero modes are detected and hence the gauge fields can be identified as carrying a certain, well defined topological charge. We show in fig. 1 three of such zero modes as a function of the Euclidean time and the taxi driver distance[20]. The modes are localized over a small space-time region on the lattice. In addition, it seems that all zero modes are concentrated on roughly the same points in the lattice.

The behavior of the zero modes and their properties are not very well understood at the moment. Studying zero modes and topology within a chiral invariant formulation of lattice QCD is a rather new and promising field which will be actively pursued in the next years. The hope is to obtain a much better insight and even a quantitative understanding of the validity of the semiclassical picture of QCD and hence on the confinement and chiral symmetry breaking phenomena.

3 Flux Tubes

Related to the discussion in the previous section, is the question, how the force is transmitted between quarks when they are confined. The generally accepted picture is the one of a flux tube that emerges when the quarks are taken apart. This leads finally to a string that is built up between the quarks with a certain string tension and a constant force between the quarks. Such a force would lead to the confinement of quarks, since any attempt to separate them would require an infinite amount of energy.

A standard setup to test such a picture in lattice simulations is to give the quarks infinite mass in order to make them static and to investigate the behavior of the gauge fields when the static quarks are put at various distances from each other.

The picture observed in real simulations can be seen in fig. 2, where we show a static quark (q) and antiquark ($\bar{q}$), separated by a distance of about one fermi, immersed in the QCD vacuum. The l.h.s. of the figure shows the color electric flux lines, while the r.h.s. shows the (solenoidal) color magnetic monopole currents. The QCD vacuum can thus be interpreted as a dual superconductor, in which the monopoles condense and, by means of a dual Meissner effect, constrict the electric flux into a narrow tube. The result is a linear confining potential acting between quark and antiquark[21].

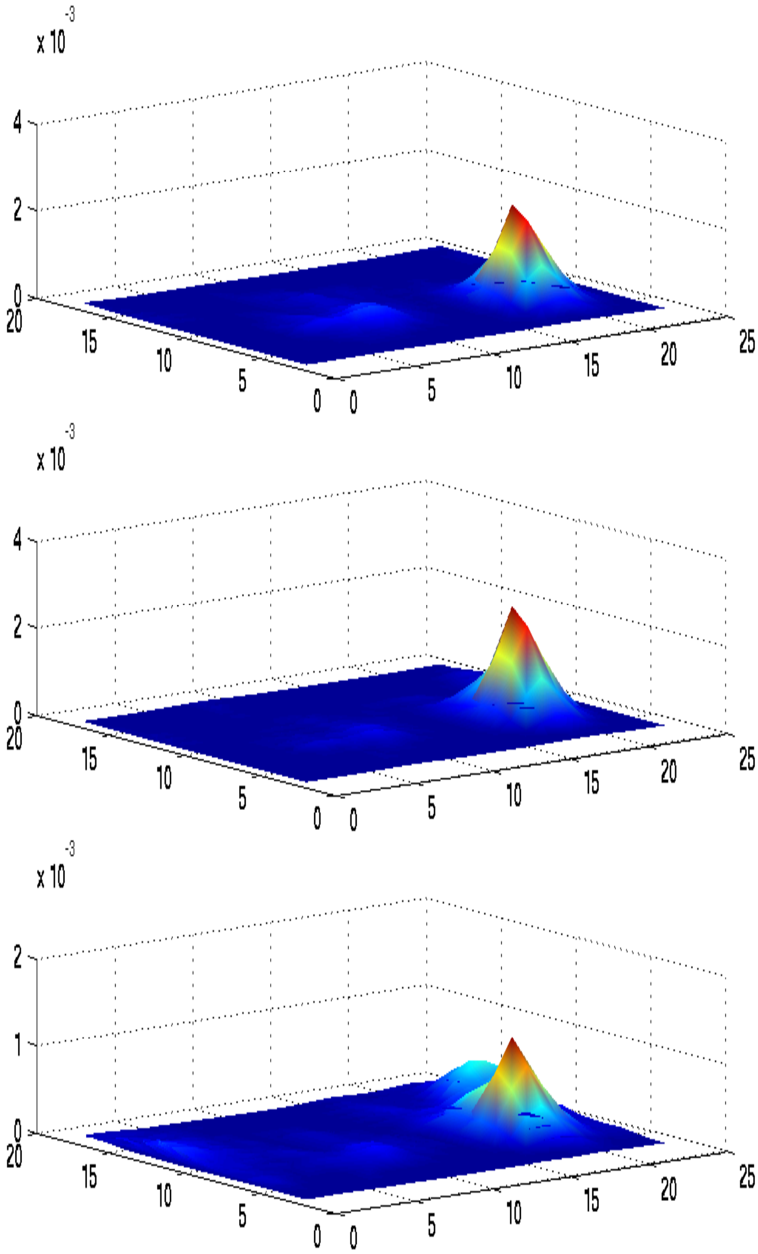

Figure 1. Three zero modes as obtained from a simulation employing Ginsparg-Wilson fermions. The modes are localized states and sit on top of each other. We plot the modes as a function of the Euclidean time and the taxi-driver distance.

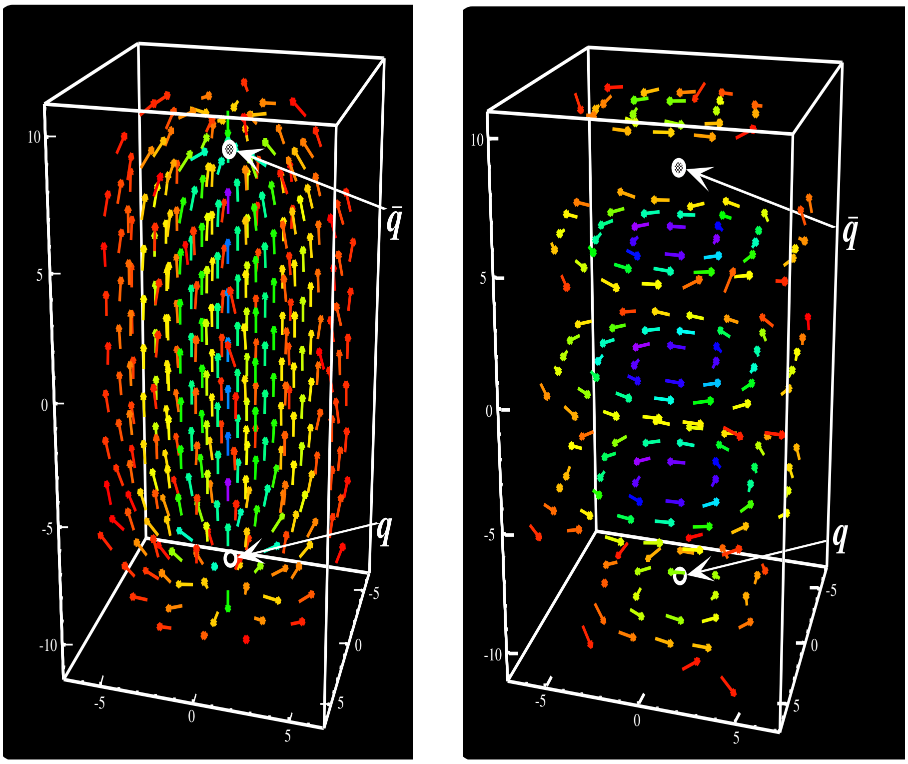

Figure 2. The color electric flux lines (left figure) and the magnetic monopole current (right figure) of a static quark-antiquark pair.

4 Various Other Results

Testing important qualitative pictures in QCD and searching for mechanisms of how, e.g. confinement or chiral symmetry breaking is realized is one aspect of lattice QCD. Another important line of research are conceptual developments such as diminishing discretization effects, utilizing finite size effects and performing non-perturbative renormalizations on which I have reported in a previous NIC proceedings contribution[22].

Of course, in order to make contact to phenomenology and experiments, quantitative predictions have to emerge from the lattice simulations. As examples for such predictions we mention here only a few.

Low-energy constants of the chiral Lagrangian

Chiral perturbation theory describes the low-energy properties of QCD[23]. It is parameterized by a number of so-called low-energy constants which cannot be determined by chiral perturbation theory itself but have to be obtained from other sources. The lattice is ideally suited for providing quantitative predictions from QCD for these low-energy constants which can eventually be compared to experimental results. The NIC group is involved in such calculations analytically[24] and numerically[25] and determined the scalar condensate, the order parameter of chiral symmetry breaking, to come out to be $\Sigma = (250\mathrm{MeV})^3$ [26–28] and the pion decay constant to be $F_\pi = 130\mathrm{MeV}$ [25].

Structure functions
The spin structure of hadrons can be parameterized by structure functions which can be related to moments of parton (quark) distribution functions. Such moments can be computed, on the one hand, directly on the lattice and, on the other hand, can be extracted from experimental data through global analyses of the world data obtained in deep inelastic scattering.

Most of the present simulations are performed in the so-called quenched approximation, where the steady generation of virtual quark anti-quark pairs are completely neglected. It turns out, however, that this approximation is surprisingly close to experimental results with an about 20% systematic effect. Of the many results that are obtained on the lattice in the quenched approximation and we only list here a few examples: the lowest moment of a pion, non-singlet parton distribution function comes out to be $\langle x \rangle = 0.265(15)$ [29]. The axial charge g_A is found to be $g_A = 1.14(3)$ [30] and moments of unpolarized quark distribution functions for the h_1 transversity structure function is $\delta u = 1.028(15)$ and the spin-dependent structure function d_2, $\Delta u = 0.889(29)$. First results in unquenched simulations with $N_f = 2$ flavors of quarks are also available and give $g_A = 1.15(7)$, $\delta u = 1.04(4)$ [30].

The next challenge is to address dynamical fermions with $2 + 1$ (two light and one heavy) flavors. It should be stressed that such calculations are in principle possible in a completely analogous way as the calculations were performed that led to the above results. The only missing ingredient is sufficient computer power. The set up of dynamical $2 + 1$ flavor simulations would give definite predictions from QCD that are to be confronted with experimental data to either confirm QCD as the correct theory of the strong interaction or to provide hints for physics beyond the standard model.

5 Algorithms and Machines

The physics projects discussed above would not be possible to perform without a continuous improvement of the algorithms employed and using high-end, powerful supercomputers.

The NIC research group is involved in the development of fermion algorithms for QCD since many years[31,32] and could achieve substantial improvements. The group also participates in testing and benchmarking computer platforms[33] and has established a benchmark suite that can be used for different architectures in order to test their applicability for lattice QCD simulations.

Another important activity of the NIC group is the development of massively parallel supercomputers, in particular the APE (Array Processor Experiment) machines[34]. APE computers are custom made and have a long history already with a first machine installed in Italy around 1985. The first machine used in the high energy physics community in Germany was the APE100. This machine appeared to be extremely successful. It is a massively parallel SIMD machine with a fast interconnecting network. APE100 ran very stable in practice and became the workhorse for many groups performing lattice gauge

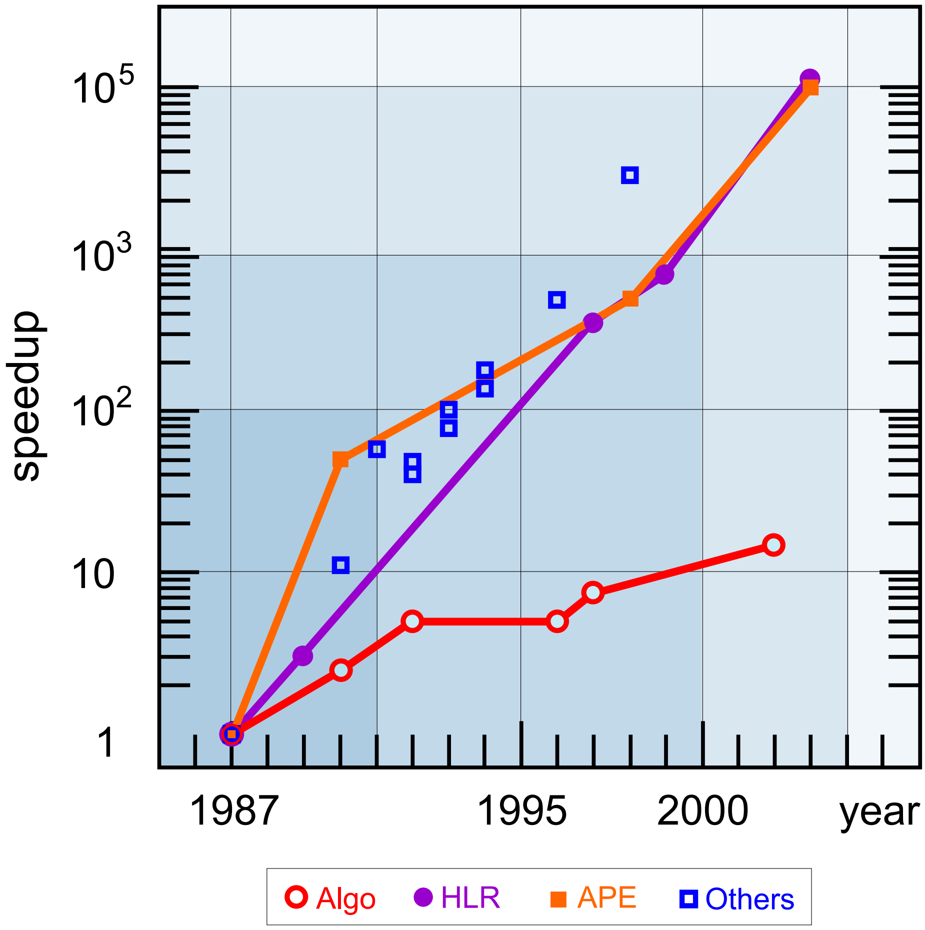

Figure 3. The relative improvement of the algorithms (algo) used in lattice gauge theory as compared to the relative increase of computer power in the last 15 years. The normalization is the year 1987, the year of birth of the Hybrid Monte Carlo algorithm, the first exact algorithm to simulate dynamical quarks. APE denotes the custom made Array Processor Experiment machines, HLR machines that were available for lattice gauge theorists at supercomputer centers, here the supercomputer center in Jülich and others denote available computer power at various places in the world.

theory simulations. The APEmille computer is the successor of APE100 and hence already the third generation of APE machines. At Zeuthen, NIC provides access to a 550Gflops installation of APEmille to the German lattice community. The machine operates very stable and has become a reliable, cheap and efficient source of computer time for lattice QCD in Germany and Europe-wide.

In fig. 3 (taken from the LATFOR proposal[35]) the algorithm improvement that could be achieved in the last 15 years is depicted. Unfortunately, no breakthrough in the algorithm development could be achieved like in other fields with the cluster algorithms in spin models[36] or recent developments for gauge theories[37]. Nevertheless, relatively small im-

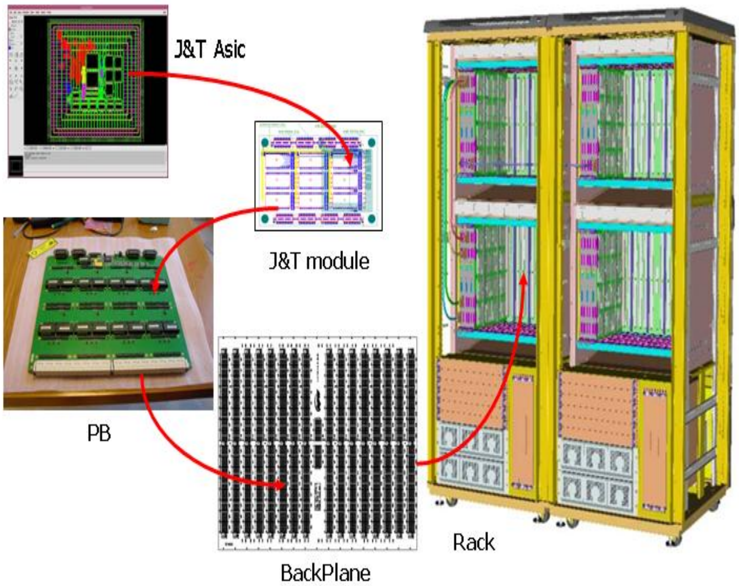

Figure 4. The design parts of the apeNEXT machine.

provements accumulated to a total gain of a factor of 20 today as compared to the situation in the year 1987, the year of birth of the first exact algorithm to simulate dynamical quarks, the hybrid Monte Carlo algorithm[38]. Note that this factor does not include other conceptual developments that come on top.

The figure also demonstrates that in the same time period, the development of powerful supercomputers has led to an orders of magnitude larger increase of computing resources. The APE machine follow essentially the line of commercial supercomputers as they were available at supercomputer centers, here the NIC at the research center Jülich. Of course, the fact that APE is a specialized machines leads to a number of advantages. They are much –an order of magnitude– cheaper, and they need less power consumption, footprint and cooling.

Following a recommendation from the Lattice Forum of German lattice physicists[35], the newest version of APE, apeNEXT will be a major source of computer power. We show in fig. 4 the main design parts of the machine, for details we refer to Ref. 34. Major differences to earlier APE machines are that apeNEXT runs in 64-bit precision while its predecessors had only 32-bit words. It is a SPMD machine and runs asynchronously giving new challenges to the APE collaboration. The final installations will achieve 2-3Tflops for a stand alone system with price/performance ratio of 0.5Euro/Mflop (peak). These parameters will then meet the requirements formulated by an ECFA panel[39] for the performance needs of lattice field theory in the next years and the LATFOR proposal[35] which evaluates a need of 25 Tflops for the physics program of the German community.

6 Conclusion

Lattice field theory has become an integral part of theoretical high energy physics. It helps to understand better the theoretical models of elementary particle physics and to test non-perturbative aspects that are of fundamental importance such as the mechanisms of confinement or chiral symmetry breaking and properties of phase transitions. Moreover, lattice calculations provide non-perturbatively obtained values for physical quantities that derive from the underlying model alone without further assumptions.

In order to obtain such results, a continuous effort is made to improve the algorithms employed in the simulations and to develop theoretical concepts such as improving on discretization errors, utilizing finite size effects and perform non-perturbative renormalizations. However, despite the progress on the algorithmic and conceptual side, powerful supercomputers are mandatory to solve the outstanding problems of dynamical and chiral invariant lattice fermions. Centers such as NIC are most suitable to satisfy this demand by providing state of the art, high-end commercial and custom made supercomputers.

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